Engineering the band structure of $Hg_{1-x}(Cd|Mn)_xTe$ with x-Cd or x-Mn component based two- and three-dimensional topological insulator

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Abstract

Since the HgTe materials were discovery as a material with topological insulator properties in two cases: so called three dimensional (3D) as well as two dimensional (2D) topological insulator (for 75nm wide and about 6.4nm wide QW HgTe films respectively for 3D ant 2D cases) many papers were devoted investigation concerning the electronics, optics and many other different properties for such structures. All of this activity, beside from the pure science point of view, were caused to know better the properties from the point of view of the possible applications region for such new state of mater based on HgTe compounds. In this papers however we present the properties much more complex structures like $A_{1-x}B_xC$ solid solutions based on HgTe (A and C) materials with different then 0 x- Cd and Mn compounds (B - part in the $Hg_{1-x}B_xTe$). Beside the differences caused by influence Cd and Mn compound into the HgTe materials the additional physical, structural and geometry factors are taking into account from the point of view of the possible properties such modified HgTe-based compounds. To show how all of these properties can by changed for such complex structures comparing with the HgTe pure materials we all our investigation presents here is flowed on the based on very well know theoretical eight band kp model which is a key to understand all of the electronic, optics and many diffident properties flowing from this state of maters. Additional magnetic field and Landau levels spectroscopy can give the information about quality of the TI states for investigated $Hg_{1-x}B_xTe$ solid solutions. Together with the physical and external conditions such as bulk inversion asymmetry (BIA), structural inversion asymmetry (SIA) and Interface inversion asymmetry (IIA) which plays critical role in the TI cases the band structure modification are also taking into account in presented paper from the point of view the modifications parameters comparing to that obtained for 3D as well as 2D materials pure HgTe films.

Theory

$$H_0 = \begin{bmatrix} T & 0 & \frac{-1}{\sqrt{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{6}}Pk_- & 0 & \frac{-1}{\sqrt{3}}Pk_z & -\frac{1}{\sqrt{3}}Pk_- \\ 0 & T & 0 & -\frac{1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{2}}Pk_- & -\frac{1}{\sqrt{3}}Pk_+ & \frac{1}{\sqrt{3}}Pk_z \\ -\frac{1}{\sqrt{2}}k_-P & 0 & U+V & -\bar{S}_- & R & 0 & \frac{1}{\sqrt{2}}\bar{S}_- & -\sqrt{2}R \\ \sqrt{\frac{2}{3}}k_zP & -\frac{1}{\sqrt{6}}k_-P & -\bar{S}_-^\dagger & U-V & C & R & \sqrt{2}V & -\sqrt{\frac{3}{2}}\tilde{S}_- \\ \frac{1}{\sqrt{6}}k_+P & \sqrt{\frac{2}{3}}k_zP & R^\dagger & C^\dagger & U-V & \bar{S}_+^\dagger & -\sqrt{\frac{3}{2}}\tilde{S}_+ & -\sqrt{2}V \\ 0 & \frac{1}{\sqrt{2}}k_+P & 0 & R^\dagger & \bar{S}_+ & U+V & \sqrt{2}R^\dagger & \frac{1}{\sqrt{2}}\bar{S}_+ \\ -\frac{1}{\sqrt{3}}k_zP & -\frac{1}{\sqrt{3}}k_-P & \frac{1}{\sqrt{2}}\bar{S}_-^\dagger & \sqrt{2}V & -\sqrt{\frac{3}{2}}\tilde{S}_+^\dagger & \sqrt{2}R & U-\Delta & C \\ -\frac{1}{\sqrt{3}}k_+P & \frac{1}{\sqrt{3}}k_zP & -\sqrt{2}R^\dagger & -\sqrt{\frac{3}{2}}\tilde{S}_-^\dagger & -\sqrt{2}V & \frac{1}{\sqrt{2}}\tilde{S}_+^\dagger & C^\dagger & U-\Delta \end{bmatrix}$$

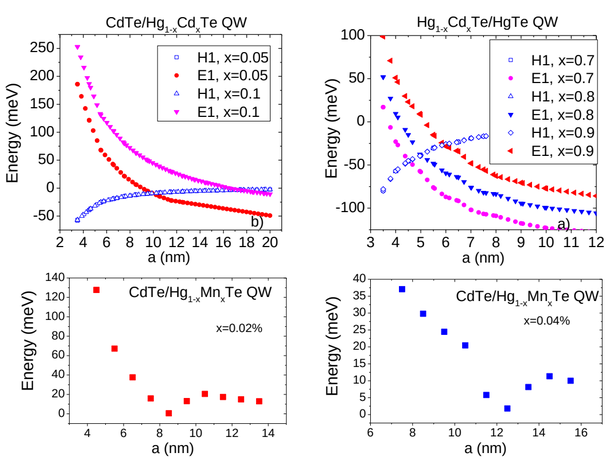
$$k_{||}^2 = k_x^2 + k_y^2, \quad k_\pm = k_x \pm ik_y, \quad k_z = -i\partial/\partial z,$$
$$T = E_c(z) + \frac{\hbar^2}{2m_0}[(2F+1)k_{||}^2 + k_z(2F+1)k_z],$$
$$U = E_v(z) - \frac{\hbar^2}{2m_0}(\gamma_1 k_{||}^2 + k_z\gamma_1 k_z),$$
$$V = -\frac{\hbar^2}{2m_0}(\gamma_2 k_{||}^2 - 2k_z\gamma_2 k_z),$$
$$R = -\frac{\hbar^2}{2m_0}\sqrt{3}(\mu k_+^2 - \bar{\gamma}k_-^2),$$
$$\bar{S}_\pm = -\frac{\hbar^2}{2m_0}\sqrt{3}k_\pm(\{\gamma_3, k_z\} + [\kappa, k_z]),$$
$$\tilde{S}_\pm = -\frac{\hbar^2}{2m_0}\sqrt{3}k_\pm\left(\{\gamma_3, k_z\} - \frac{1}{3}[\kappa, k_z]\right),$$
$$C = \frac{\hbar^2}{m_0}k_-[\kappa, k_z].$$

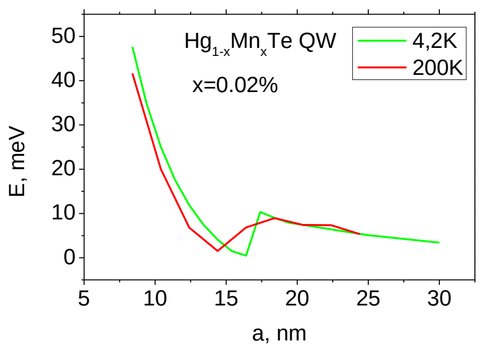
TABLE I. Band structure parameters of HgTe and CdTe (Refs.[?,?]).

	HgTe	CdTe		HgTe	CdTe
E_g	-0.303 eV	1.606 eV	C	-3.83 eV	-4.06 eV
E_v	0	-570 meV	a	0	-0.7 eV
Δ	1.08 eV	0.91 eV	b	-1.5 eV	-1.17 eV
E_p	18.8 eV	18.8 eV	d	-2.08 eV	-3.2 eV
F	0	-0.09	C_{11}	53.6 GPa	53.6 GPa
γ_1	4.1	1.47	C_{12}	36.6 GPa	37.0 GPa
γ_2	0.5	-0.28	C_{44}	21.2 GPa	19.9 GPa
γ_3	1.3	0.03			
κ	-0.4	-1.31			

3D, 2D Hg(Cd|Mn)Te

$$(H_0 + H_{BP} + V(z))\Psi(z) = E\Psi(z)$$





3D, 2D HgCdTe with assymetry

$$(H_0 + H_{BP} + H_{SIA} + H_{BIA} + H_{IIA} + V(z))\Psi(z) = E\Psi(z)$$